Modeling and Prediction Using Stochastic Differential Equations

Pharmacokinetic/pharmakodynamic (PK/PD) modeling for a single subject is most often performed using nonlinear models based on deterministic ordinary differential equations (ODEs), and the variation between subjects in a population of subjects is described using a population (mixed effects) setup that describes the variation between subjects. The ODE setup implies that the variation for a single subject is described by a single parameter (or vector), namely the variance (covariance) of the residuals. Furthermore the prediction of the states is given as the solution to the ODEs and hence assumed deterministic and can predict the future perfectly. A more realistic approach would be to allow for randomness in the model due to e.g., the model be too simple or errors in input. We describe a modeling and prediction setup which better reflects reality and suggests stochastic differential equations (SDEs) for modeling and forecasting. It is argued that this gives models and predictions which better reflect reality. The SDE approach also offers a more adequate framework for modeling and a number of efficient tools for model building. A software package (CTSM-R) for SDE-based modeling is briefly described.

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